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Investigation of Temperature Dependence Thermoelectric Figure of Merit (ZT) in Low-dimensional Bi_2Te_3

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Abstract: In this study, mathematical calculation of thermoelectric figure of merit (ZT) has been derived in low-dimensional semiconductor materials on the based on density of states for quantum systems. The quantum mechanical behavior, temperature and size dependent of these nanostructures have been described more completely.

Key words: Thermoelectric, semiconductor, figure of merit, low-dimensional systems, nanostructures

INTRODUCTION

In this study, mathematical calculation of thermoelectric figure of merit (ZT) has been derived in low-dimensional semiconductor materials on the based on density of states for quantum systems. The quantum mechanical behavior, temperature and size dependent of these nanostructures have been described more completely. The study of thermoelectric phenomena in semiconductor materials is not new; it does back to Seebeck's works in the years 1821-1823 (Treatise, 2001a). However, within recent years has been renewed and intensive study of thermoelectric effect (Carotenuto *et al*., 2009; Heremans and Thrush, 1999) due to realization of the need both experimentally and theoretically to study more behavior of thermoelectric materials (Glatz and Beloborodov, 2009; Radwan, 2001). Generation of nanostructure materials for thermoelectric applications has attracted great interest in recent years because of their high efficiencies and unique physical properties which are different from those of either the bulk materials (Goldsmid, 1964; Treatise, 2001a; Zheng, 2008). The efficiency of thermoelectric power for a material is usually made in terms of dimensionless figure of merit (ZT) defined by Carotenuto *et al*. (2009), Heremans and Thrush (1999), Miller (2000), Treatise (2001a), Senthilkumaar and Thamiz Selvi (2008), Zheng (2008) and Zhang *et al*. (2009):

$$ZT = \frac{\sigma S^2 T}{\kappa_e + \kappa_{ph}} \quad (1)$$

where, S is the see beck coefficient, σ is the electrical conductivity, T is the temperature (Kelvin), κ_{ph} is the phonon thermal conductivity and κ_e is the electronic thermal conductivity. In order to achieve high thermoelectric performance (or high ZT), one requires a high thermoelectric power S, where S denotes the voltage generated by thermal gradient, a high electrical conductivity (σ) and low thermal conductivity (κ_e+κ_{ph}). Since an increase in S for a typical material leads to a decrease in σ, due to carrier density consideration and an increase in σ leads to an increase in the electronic contribution to κ_e+κ_{ph}, so, it is very difficult to increase Z in typical thermoelectric materials (Malyarevich *et al*., 2007; Heremans and Thrush, 1999; Zhang *et al*., 2009).

Confinement of charge carriers in a nanometer scale thermoelectric materials increases the local carrier density of states per unit volume near the Fermi energy increasing the see beck coefficient (Treatise, 2001a, b; Bhushan, 2007), while the thermal conductivity can be decreased due to phonon confinement (Bhandari, 1995; Muller, 2005; Liu *et al*., 2008; Zhang and Xu, 2008; Pendyala and Rao, 2009) and phonon scattering at the material interfaces in nanostructures. In the present work, we describe the temperature and size dependence of thermoelectric efficiency (ZT) in Bi_2Te_3 nanostructures (Treatise, 2001c; Naves *et al*., 2006; Boberl *et al*., 2008).

THEORY

At first we need to calculate electrical conductivity (σ), electronic thermal conductivity (κ_e) and Seebeck coefficient (S) for 1D, 2D and 3D nanostructures.

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Calculation of electrical conductivity for 1D, 2D and 3D: Whit definition of distribution function of Fermi-Dirac f_0 and integral of Fermi and density of state g (E), we calculate electrical conductivity for 1D, 2D, 3D as follows (Muller, 2005):

$$\sigma = -2\frac{e^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g\,(E)E\tau dE \qquad (2)$$

Where:

$$f_0 = \frac{1}{1+e^{\frac{E-E_F}{K_BT}}}$$

$$\tau = \frac{m\mu}{e}$$

Fermi integral is:

$$F_n = \int_0^{\infty}\frac{x^n dx}{1+e^{x-\frac{E_F}{K_BT}}}$$

and density of state for 3D:

$$g_{3D}(E) = \frac{\sqrt{m_x m_y m_z}}{\pi^2\hbar^3}\sqrt{2E}$$

With substitute in relation 2 for 3D we have:

$$\sigma_{3D} = -2\frac{e^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}\frac{(2m)^{3/2}}{2\pi^2\hbar^3}\sqrt{E}E\tau dE$$

where, $m = (m_x m_y m_z)^{3/2}$, therefore:

$$\sigma_{3D} = \frac{e}{2}\frac{(2m)^{3/2}}{\pi^2\hbar^3}\mu\,(K_BT)^{3/2}\int_0^{\infty}\frac{x^{1/2}}{1+e^{x-\frac{E_F}{K_BT}}}dx \qquad (3)$$

and by definition of F_n we have:

$$\sigma_{3D} = \frac{1}{2\pi^2}(\frac{2K_BT}{\hbar^2})^{3/2}\mu.em^{3/2}F_{1/2}$$

Then:

$$\sigma_{3D} = \frac{1}{2\pi^2}(\frac{2K_BT}{\hbar^2})^{3/2}\mu e\sqrt{m_x m_y m_z}F_{1/2} \qquad (4)$$

Now, for achieve electrical conductivity 1D and 2D, we use from Wiedemann-Franz's law $\sigma = n_{iD}e\mu$, where i = 1, 2, 3:

$$n_{iD} = \int_{E=0}^{\infty}g_{iD}(E)f_0(E)dE \qquad (5)$$

And:

$$g_{2D}(E) = \frac{\sqrt{m_x m_y}}{\pi\hbar^2 d} \qquad (6)$$

With substitute f_0 and density of state 2D at Eq. 6 we have:

$$n_{2D} = \int_{E=0}^{\infty}\frac{m}{\pi\hbar^2 d}\frac{1}{1+e^{\frac{E-E_F}{K_BT}}}dE = \frac{m}{\pi\hbar^2 d}\int_{E=0}^{\infty}\frac{1}{1+e^{\frac{E-E_F}{K_BT}}}dE \qquad (7)$$

where, $m = \sqrt{m_x m_y}$, therefore:

$$n_{2D} = \frac{\sqrt{m_x m_y}}{\pi\hbar^2 d}\int_0^{\infty}\frac{1}{1+e^{x-\frac{E_F}{K_BT}}}K_BTdx = \frac{1}{\pi d}(\frac{K_BT}{\hbar^2})\sqrt{m_x m_y}\int_0^{\infty}\frac{1}{1+e^{x-\frac{E_F}{K_BT}}}dx$$

Therefore, from definition F_n, we have:

$$n_{2D} = \frac{1}{\pi d}(\frac{2K_BT}{\hbar^2})\sqrt{m_x m_y}F_0 \qquad (8)$$

Finally:

$$\sigma_{2D} = ne\mu = \frac{1}{2\pi d}(\frac{2K_BT}{\hbar^2})\sqrt{m_x m_y}e\mu F_0 \qquad (9)$$

Similarly, for achieve electrical conductivity 1D with substitute f_0 and:

$$g_{1D}(E) = \frac{1}{\pi^2}(\frac{2m_x}{\hbar^2})^{1/2}\frac{1}{\sqrt{E}} \qquad (10)$$

and:

$$n_{1D} = \int_{E=0}^{\infty}\frac{1}{\pi d^2}(\frac{2m}{\hbar^2})^{1/2}\frac{1}{\sqrt{E}}\frac{1}{1+e^{\frac{E-E_F}{K_BT}}}dE = \frac{1}{\pi d^2}(\frac{2m}{\hbar^2})^{1/2}\int_{E=0}^{\infty}\frac{1}{\sqrt{E}}\frac{1}{1+e^{\frac{E-E_F}{K_BT}}}dE \qquad (11)$$

where, $m = m_x$, therefore:

$$n_{1D} = \frac{1}{\pi d^2}(\frac{2m}{\hbar^2})^{1/2}\int_0^{\infty}\frac{1}{\sqrt{K_BTx}}\frac{1}{1+e^{x-\frac{E_F}{K_BT}}}K_BTdx = \sqrt{K_BT}\frac{1}{\pi d^2}(\frac{2m}{\hbar^2})^{1/2}\int_0^{\infty}\frac{x^{-1/2}}{1+e^{x-\frac{E_F}{K_BT}}} \qquad (12)$$

$$= \frac{1}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\sqrt{m_x}F_{-1/2} \qquad (13)$$

by relation Eq. 5 we have:

$$\sigma_{1D} = ne\mu = \frac{1}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\sqrt{m_x}e\mu F_{-1/2} \qquad (14)$$

Calculation of thermal conductivity (κ_e) for 1D, 2D and 3D: For calculate thermal conductivity 3D we substitute f_0, τ and density of state 3D in relation:

$$\kappa_e = \frac{2}{3m_xT}\left\{\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{3D}(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{3D}(E)E\tau dE} - \int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{3D}(E)E^3\tau dE\right\} \qquad (15)$$

We have:

$$\kappa_e = \frac{2}{3m_xT}\left\{\frac{\frac{25}{4}(K_BT)^5\tau^2\left(\frac{1}{2\pi^2}\right)^2\left(\frac{2m}{\hbar^2}\right)^3F_{3/2}^2}{-\frac{3}{2}(K_BT)^{3/2}\tau\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}F_{1/2}} + \frac{7}{2}(K_BT)^{7/2}\tau\frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}F_{5/2}\right\}$$
$$= \frac{2}{3m_xT}\frac{\tau}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}(K_BT)^{7/2}\left\{\frac{7}{2}F_{5/2} - \frac{25F_{3/2}^2}{6F_{1/2}}\right\} \qquad (16)$$

where, $m^{3/2} = \sqrt{m_xm_ym_z}$. Therefore, thermal conductivity for 3D is:

$$\kappa_e = \frac{\tau\hbar^2}{6\pi^2}\left(\frac{2K_BT}{\hbar^2}\right)^{5/2}\left(\frac{m_ym_z}{m_x}\right)^{1/2}K_B\left\{\frac{7}{2}F_{5/2} - \frac{25F_{3/2}^2}{6F_{1/2}}\right\} \qquad (17)$$

Now for calculation thermal conductivity 1D, 2D from Wiedemann-Franz's law we have:

$$\kappa_e = \frac{2}{m_xT}\left\{\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{2D}(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{2D}(E)E\tau dE} - \int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{2D}(E)E^3\tau dE\right\} \qquad (18)$$

Hence, for thermal conductivity 2D with notation to g_{2D} (E) and other supposition we have:

$$\kappa_e = \frac{2}{m_xT}\left\{\frac{4\tau^2\left(\frac{m}{\pi\hbar^2}\right)^2\left(\frac{1}{d}\right)^2(K_BT)^4F_1^2}{-\tau\frac{m}{\pi\hbar^2}\frac{1}{d}(K_BT)F_0} + 3\tau\frac{m}{\pi\hbar^2}\frac{1}{d}(K_BT)^3F_2\right\} \qquad (19)$$
$$= \frac{2}{m_xT}\frac{m\tau}{\pi\hbar^2 d}(K_BT)^3\left\{3F_2 - \frac{4F_1^2}{F_0}\right\}$$

where, $m = \sqrt{m_xm_y}$. Therefore, thermal conductivity 2D is:

$$\kappa_e = \frac{\tau\hbar^2}{4\pi d}\left(\frac{2K_BT}{\hbar^2}\right)^2\left(\frac{m_y}{m_x}\right)^{1/2}K_B\left\{3F_2 - \frac{4F_1^2}{F_0}\right\} \qquad (20)$$

Now, for 1D, we have:

$$\kappa_e = \frac{2}{m_xT}\left\{\frac{\left(\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{1D}(E)E^2\tau dE\right)^2}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{1D}(E)E\tau dE} - \int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g_{1D}(E)E^3\tau dE\right\} \qquad (21)$$

Therefore:

$$\kappa_e = \frac{2}{m_xT}\left\{\frac{\frac{9}{4}(K_BT)^3\tau^2\frac{1}{\pi^2d^4}\frac{2m}{\hbar^2}F_{1/2}^2}{-\frac{1}{2}(K_BT)^{1/2}\tau\frac{1}{\pi d^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}F_{-1/2}} + \frac{5}{2}(K_BT)^{5/2}\tau\frac{1}{\pi d^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}F_{3/2}\right\}$$
$$= \frac{2}{m_xT}(K_BT)^{5/2}\tau\frac{1}{\pi d^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\left\{\frac{5}{2}F_{3/2} - \frac{9F_{1/2}^2}{2F_{-1/2}}\right\} \qquad (22)$$

That $m = m_x$. Then finally:

$$\kappa_e = \frac{2\tau}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}m_x^{-1/2}K_B^2T\left\{\frac{5}{2}F_{3/2} - \frac{9F_{1/2}^2}{2F_{-1/2}}\right\} \qquad (23)$$

Calculation of Seebeck coefficient (S) for 1D, 2D and 3D: For calculate Seebeck coefficient we use from following relation:

$$S = \frac{\frac{2e}{3mT}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g(E)E(E-\mu)\tau dE}{-\frac{2e^2}{3m}\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g(E)E\tau dE} = \frac{-1}{eT}\left(\frac{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g(E)E^2\tau dE}{\int_{E=0}^{\infty}\frac{\partial f_0}{\partial E}g(E)E\tau dE}\right. \qquad (24)$$

for calculate Seebeck coefficient for 3D with notation to F_n and f_0 and g_{3D} we have:

$$S_{3D} = \frac{1}{-eT}\left(\frac{-5/2\frac{(2m)^{3/2}\tau}{2\pi^2\hbar^3}(K_BT)^{5/2}F_{3/2}}{-3/2\frac{(2m)^{3/2}}{2\pi^2\hbar^3}\tau(K_BT)^{3/2}F_{1/2}} - \mu\right) \qquad (25)$$
$$= \frac{1}{-eT}\left(\frac{5K_BTF_{3/2}}{3F_{1/2}} - \mu\right) = -\frac{K_B}{e}\left(\frac{5F_{3/2}}{3F_{1/2}} - \frac{\mu}{K_BT}\right)$$

$$= -\frac{K_B}{e}\left(\frac{5F_{3/2}}{3F_{1/2}} - \xi^*\right) \qquad (26)$$

Where:

$$\xi^* = \frac{\mu}{K_BT}$$

Now for achieve Seebeck coefficient 2D with iteration up stages and relation Eq. 25 we have:

$$S_{2D}=\frac{1}{-eT}\left(\frac{-\frac{2m\tau}{\pi\hbar^2 d}(K_BT)^2F_1}{-\frac{m}{\pi\hbar^2 d}\tau(K_BT)F_0}-\mu\right)=\frac{1}{-eT}\left(\frac{2K_BTF_1}{F_0}-\mu\right)=-\frac{K_B}{e}\left(\frac{2F_1}{F_0}-\frac{\mu}{K_BT}\right)=-\frac{K_B}{e}\left(\frac{2F_1}{F_0}-\xi^*\right)\tag{27}$$

Similarly, for 1D, we can achieve as follows:

$$S_{1D}=\frac{1}{-eT}\left(\frac{-\frac{3}{2}\frac{1}{2\pi d^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\tau(K_BT)^{3/2}F_{1/2}}{-\frac{1}{2}\frac{1}{2\pi d^2}\left(\frac{2m}{\hbar^2}\right)^{1/2}\tau(K_BT)^{1/2}F_{-1/2}}-\mu\right)=\frac{1}{-eT}\left(\frac{3K_BTF_{1/2}}{F_{-1/2}}-\mu\right)=-\frac{K_B}{e}\left(\frac{3F_{1/2}}{F_{-1/2}}-\frac{\mu}{K_BT}\right)=-\frac{K_B}{e}\left(\frac{3F_{1/2}}{F_{-1/2}}-\xi^*\right)\tag{28}$$

Calculation of figure of merit (ZT) for 1D, 2D and 3D: By substitution of Eq. 14, 23 and 28 in relation (Eq. 1) we have:

$$Z_{1D}T=\frac{\frac{1}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\sqrt{m_x}e\mu_xF_{-1/2}\frac{K_B^2}{e^2}\left(\frac{3F_{1/2}}{F_{-1/2}}-\xi^*\right)^2T}{\frac{2\tau}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{m_x}}K_B^2T\left(\frac{5}{2}F_{3/2}-\frac{9F_{1/2}^2}{2F_{-1/2}}\right)+\kappa_{ph}}$$
$$=\frac{\frac{1}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\sqrt{m_x}e\mu_xF_{-1/2}\frac{K_B^2}{e^2}\left(\frac{3F_{1/2}}{F_{-1/2}}-\xi^*\right)^2T}{\frac{2\tau}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{m_x}}K_B^2T\left[\left(\frac{5}{2}F_{3/2}-\frac{9F_{1/2}^2}{2F_{-1/2}}\right)+\kappa_{ph}\left(\frac{\pi d^2}{2\tau}\left(\frac{\hbar^2}{2K_BT}\right)^{1/2}\sqrt{m_x}\frac{1}{K_B^2T}\right)\right]}\tag{29}$$

By simplification we can write:

$$Z_{1D}T=\frac{\frac{1}{e}m_x\mu_xF_{-1/2}\left(\frac{3F_{1/2}}{F_{-1/2}}-\xi^*\right)^2}{2\frac{\mu_xm_x}{e}\left[(5/2F_{3/2}-\frac{9F_{1/2}^2}{2F_{-1/2}})+\frac{\pi d^2\kappa_{ph}\sqrt{m_x}}{2\tau K_B^2T}\left(\frac{\hbar^2}{2K_BT}\right)^{1/2}\right]}=\frac{1/2\left(\frac{3F_{1/2}}{F_{-1/2}}-\xi^*\right)F_{-1/2}}{\frac{1}{B_{1D}}+\left(5/2F_{3/2}-\frac{9F_{1/2}^2}{2F_{-1/2}}\right)}\tag{30}$$

Where:

$$B_{1D}=\frac{2}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\frac{K_B^2T\sqrt{m_x}\mu_x}{e\kappa_{ph}}\tag{31}$$

But since in calculation ZT in 1D, six charge carrier supposed, therefore, B_{1D} becomes as follows:

$$B_{1D}=6\frac{2}{\pi d^2}\left(\frac{2K_BT}{\hbar^2}\right)^{1/2}\frac{K_B^2T\sqrt{m_x}\mu_x}{e\kappa_{ph}}\tag{32}$$

For calculate ZT in 2D, similarly to 1D, by substitution of relations Eq. 9, 20 and 27 in Eq. 1 we have:

$$Z_{2D}T=\frac{\frac{1}{2\pi d}\left(\frac{2K_BT}{\hbar^2}\right)\sqrt{m_xm_y}F_0e\mu_xT\frac{K_B^2}{e^2}\left(\frac{2F_1}{F_0}-\xi^*\right)^2}{\kappa_{ph}+\frac{\tau\hbar^2}{4\pi d}\left(\frac{2K_BT}{\hbar^2}\right)^2\sqrt{\frac{m_y}{m_x}}K_B\left(3F_2-\frac{4F_1^2}{F_0}\right)}$$
$$=\frac{\frac{1}{2\pi d}\left(\frac{2K_BT}{\hbar^2}\right)\sqrt{m_xm_y}F_0e\mu_xT\frac{K_B^2}{e^2}\left(\frac{2F_1}{F_0}-\xi^*\right)^2}{\frac{\tau\hbar^2}{4\pi d}\left(\frac{2K_BT}{\hbar^2}\right)^2\sqrt{\frac{m_y}{m_x}}K_B\left[\left(3F_2-\frac{4F_1^2}{F_0}\right)+\frac{4\pi d\sqrt{m_x}\kappa_{ph}}{\tau\hbar^2\sqrt{m_y}K_B}\left(\frac{\hbar^2}{2K_BT}\right)^2\right]}$$
$$=\frac{\mu_xT\frac{K_B}{e}m_xF_0\left(\frac{2F_1}{F_0}-\xi^*\right)^2}{\frac{\mu_xm_x}{e}K_BT\left(\left(3F_2-\frac{4F_1^2}{F_0}\right)+\frac{4\pi d\sqrt{m_x}\kappa_{ph}}{\tau\hbar^2\sqrt{m_y}K_B}\left(\frac{\hbar^2}{2K_BT}\right)^2\right)}=\frac{F_0\left(\frac{2F_1}{F_0}-\xi^*\right)^2}{\left(3F_2-\frac{4F_1^2}{F_0}\right)+\frac{1}{B_{2D}}}\tag{33}$$

Where:

$$\frac{1}{B_{2D}}=\frac{4\pi d\sqrt{m_x}\kappa_{ph}}{\frac{\mu_xm_x}{e}\hbar^2\sqrt{m_y}K_B}\left(\frac{\hbar^2}{2K_BT}\right)^2$$

Then:

$$B_{2D}=\frac{1}{2\pi d}\left(\frac{2K_BT}{\hbar^2}\right)\sqrt{m_xm_y}\frac{\mu_xK_B^2T}{e\kappa_{ph}}\tag{34}$$

For calculate ZT in 3D similarly to two considered cases, we substitute relations Eq. 4, 17 and 26 in Eq. 1 and so:

$$Z_{3D}T=\frac{\frac{1}{2\pi^2}\left(\frac{2K_BT}{\hbar^2}\right)^{3/2}\sqrt{m_xm_ym_z}F_{1/2}e\mu_xT\frac{K_B^2}{e^2}\left(\frac{5F_{3/2}}{3F_{1/2}}-\xi^*\right)^2}{\kappa_{ph}+\frac{\tau\hbar^2}{6\pi^2}\left(\frac{2K_BT}{\hbar^2}\right)^{5/2}\sqrt{\frac{m_ym_z}{m_x}}K_B\left(\frac{7}{2}F_{5/2}-\frac{25F_{3/2}^2}{6F_{1/2}}\right)}$$
$$=\frac{\frac{1}{2\pi^2}\left(\frac{2K_BT}{\hbar^2}\right)^{3/2}\sqrt{m_xm_ym_z}F_{1/2}e\mu_xT\frac{K_B^2}{e^2}\left(\frac{5F_{3/2}}{3F_{1/2}}-\xi^*\right)^2}{\frac{\tau\hbar^2}{6\pi^2}\left(\frac{2K_BT}{\hbar^2}\right)^{5/2}\sqrt{\frac{m_ym_z}{m_x}}K_B\left[\left(\frac{7}{2}F_{5/2}-\frac{25F_{3/2}^2}{6F_{1/2}}\right)+\frac{6\pi^2\kappa_{ph}}{\tau\hbar^2K_B}\left(\frac{\hbar^2}{2K_BT}\right)^{5/2}\left(\frac{m_x}{m_ym_z}\right)^{1/2}\right]}$$
$$=\frac{m_xF_{1/2}\mu_xT\frac{K_B}{e}\left(\frac{5F_{3/2}}{3F_{1/2}}-\xi^*\right)^2}{\frac{\mu_xm_x}{e}\frac{\hbar^2}{3}\frac{2K_BT}{\hbar^2}\left(\frac{1}{B_{3D}}+\left(\frac{7}{2}F_{5/2}-\frac{25F_{3/2}^2}{6F_{1/2}}\right)\right)}=\frac{\frac{3}{2}F_{1/2}\left(\frac{5F_{3/2}}{3F_{1/2}}-\xi^*\right)^2}{\frac{1}{B_{3D}}+\left(\frac{7}{2}F_{5/2}-\frac{25F_{3/2}^2}{6F_{1/2}}\right)},\tag{35}$$

Where:

$$\frac{1}{B_{3D}}=\frac{6\pi^2\kappa_{ph}}{\frac{m_x\mu_x}{e}\hbar^2K_B}\left(\frac{\hbar^2}{2K_BT}\right)^{5/2}\sqrt{\frac{m_x}{m_ym_z}}$$

Then:

$$B_{3D} = \frac{1}{6\pi^2}\frac{\frac{m_x\mu_x}{e}\hbar^2 K_B}{\kappa_{ph}}\left(\frac{2K_BT}{\hbar^2}\right)^{3/2}\left(\frac{2K_BT}{\hbar^2}\right)\frac{\sqrt{m_y m_z}}{\sqrt{m_x}}$$
$$= \frac{1}{3\pi^2}\frac{\frac{m_x\mu_x}{e}K_B}{\kappa_{ph}}\left(\frac{2K_BT}{\hbar^2}\right)^{3/2}\left(\frac{K_BT}{1}\right)\frac{\sqrt{m_y m_z}}{\sqrt{m_x}} \quad (36)$$
$$= \frac{1}{3\pi^2}\frac{\mu_x K_B^2 T}{e\kappa_{ph}}\left(\frac{2K_BT}{\hbar^2}\right)^{3/2}\sqrt{m_x m_y m_z}$$

DISCUSSION

By using the above mentioned theoretical expression of thermoelectric figure of merit and Seebeck constant the size and temperature dependent of these factors has been investigation at low-dimensional quantum systems. The results presented in Fig. 1, in the case of a 1-dimensional Bi_2Te_3 semiconductor crystal.

Due to differences of effective masses in a rectangular directions in Bi_2Te_3 crystals, the temperature and size dependent properties will be different in each of this direction, this is also clear in the figure.

The behavior of thermoelectric figure of merit (ZT) with different quantum sizes and temperatures in all directions of effective masses (m_x, m_y, m_z) are same but the quantities are different. The amounts of (ZT) for m_z are smaller than m_y and also the cases of m_y are smaller than m_x. The amounts of ZT in the case of m_x are large the temperature dependent of ZT are also identified for all cases. The results shows an increase in (ZT) with increase in temperature in directions of m_x, m_y and m_z it is appear from figures and observation, with increase in temperature, it will be occur an overlap between, m_x, m_y and m_z, under special temperature higher than 1000 K actually in this case we assume a fix temperature for m_y and a variable temperature for m_z. This claim presented in Fig. 2. Obviously the overlap between m_x and m_z will occur in temperature 4550 K. In the case of 1-dimensional Bi_2Te_3 nanowiers.

Calculation of 2-dimensional quantum systems were presented in, using Eq. 33. Figure 3 shows the size and temperature dependent of thermoelectric. Figure of merit (ZT) in 2-dimensional Bi_2Te_3 semiconductor crystal. Due to existence of 2-dimensional in well like system or thin films, the number of cases to be consider for this systems are in the form of m_ym_z, m_xm_z and m_xm_y. The behavior of thermoelectric figure of merit (ZT) by varying of temperatures and sizes, are similar to 1-dimensional cases. In these cases also we come control and optimized the

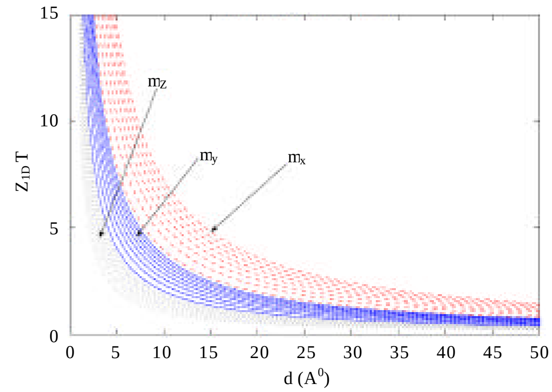

Fig. 1: Merit Z_{1D} T for Bi_2Te_3 in T = 300,..., 1000

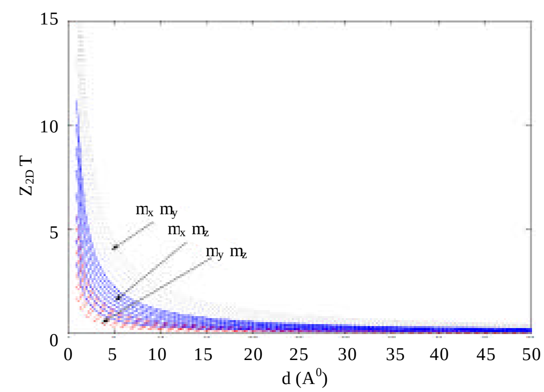

Fig. 2: Merit Z_{2D} T for Bi_2Te_3 in T = 300,..., 1000

amount of ZT by size and temperature. It is clear from Fig. 3, the maximum thermoelectric figure of merit (ZT) obtained in the case of m_xm_y direction, the smallest figure of merit (ZT) obtained in the case of m_ym_z directions.

Comparative studies between Fig. 1 and 2 shows the variation of thermoelectric figure of merit with different quantum sizes and temperature are similar and parabolic in nature but the amount of sharpness in curves (bending) are different each other and this phenomena confirms that the quantum size effect in 1-dimensional systems (quantum wires) are effective and sharp at very small sizes (sizes less than 5 nm). However in the case of 2-dimensional systems, this effect is weak. It means that the quantum size effect occurs in such size and dimensions. The quantum size effect in quantum wires more intensive to size of system and this is refer to the quantum nature of 1-dimensional systems. For bulk

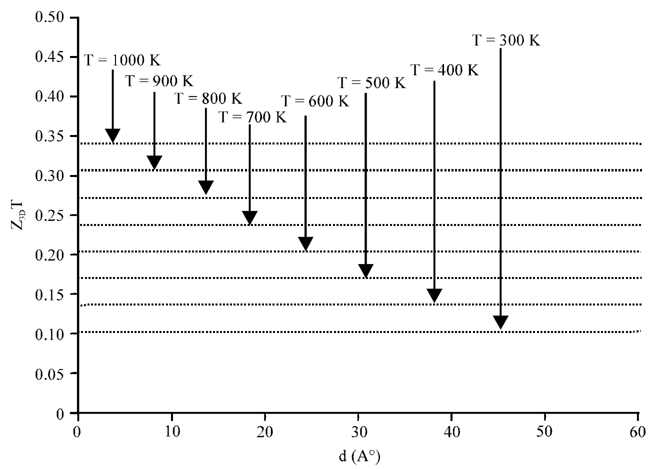

Fig. 3: Merit $Z_{3D}T$ for Bi_2Te_3 in T = 300,..., 1000 K

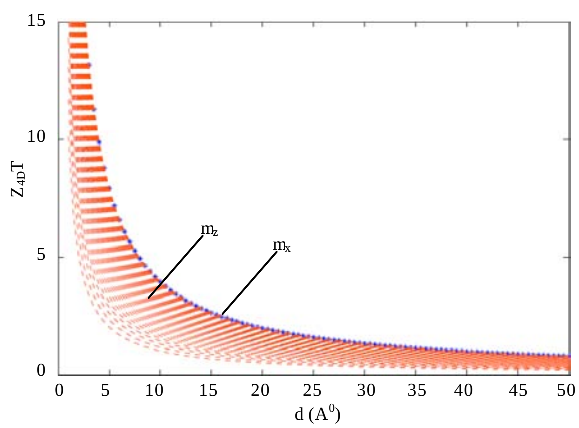

Fig. 4: Merit $Z_{4D}T$ for Bi_2Te_3 in T = 3000,..., 4550, T = 300 K for m_x and T = 300,..., 4550 K for m_z

systems, the behavior of thermoelectric materials is linear. As shown in Fig. 4 the behavior of thermoelectric figure of merit (ZT) are completely classical nature, also the influence of temperature in this case are classical but the thermoelectric figure of merit (ZT) increase by temperature (Fig. 4).

CONCLUSION

In this research, the theory of size and temperature dependent of thermoelectric figure of merit (ZT) in low-dimensional Bi_2Te_3 semiconductor crystals have been investigated. Analysis of observation shows that, the general behaviors in (ZT) at different low-dimensional are same and shows quantum mechanical nature and completely differs from its bulk behavior. Size and temperature dependent of (ZT) identifies that the quantum mechanical behavior of in the case of 2 and 1-dimensional depends on the size of systems. In the case of 1-dimensional systems, the quantum matters observed in comparison of 2-dimensional systems.

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